Large thermoelectric figure of merit for 3D topological Anderson insulators via line dislocation engineering

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We study the thermoelectric properties of three-dimensional topological Anderson insulators with line dislocations. We show that at high densities of dislocations the thermoelectric figure of merit ZT can be dominated by one-dimensional topologically-protected conducting states channeled through the lattice screw dislocations in the topological insulator materials with a non-zero time-reversal-invariant momentum such as $Bi_{1-x}Sb_x$. When the chemical potential does not exceed much the mobility edge the ZT at room temperatures can reach large values, much higher than unity for reasonable parameters, hence making this system a strong candidate for applications in heat management of nano-devices.

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Introduction. The recent crisis of heat management in nano-devices, which has lead to a lack of progression in clock speeds of charge-based logic devices, has intensified the interest in efficient thermoelectric materials. In the last decade there has been a lot of research both theoretical [1–5] and experimental [6–8] to create efficient thermoelectric nano-devices. The efficiency of such materials, which must be both p-type and n-type, is determined by a balance to convert charge flow into efficient heat transport as well as maintaining a temperature gradient between the device and the heat sink. Among the most well known thermoelectric materials in present day commercial applications one finds Bi_2Te_3, PbTe, and PbSb. These type of insulators or semiconductors have been identified recently as topological insulators (TI) [9] which exhibit protected delocalized surface states.

In the two-dimensional version of the TIs, the quantum spin Hall systems [10, 11], these protected edge states contribute to the thermoelectric efficiency but do not enhance it dramatically beyond present day materials whose efficiency parameter, ZT (see below), is of 1 or slightly less [2]. On the other hand, for three-dimensional (3D) topological insulators with a non-zero time-reversal-invariant momentum [12] (TRIM) it has been shown theoretically that one-dimensional (1D) topologically protected modes can exist in the bulk propagating through certain line dislocations [13]. These type of 1D quantum modes have been recently attributed to the results of recent experiments on Bi_2Se_3 [14, 15].

Here we explore the idea of using these 1D topologically protected modes to significantly increase the thermoelectric efficiency of materials such that $Bi_{1-x}Sb_x$, see Fig. 1. The basic premise of the proposal is to introduce, through growth engineering, a finite density of screw dislocations. This would induce disorder in the bulk leading to a reduction of the thermal conductivity, Anderson localization of bulk states, and an increase of the conductivity and thermopower contributions from these 1D states. This combination of factors, as shown below, leads to a dramatic enhancement of the figure of merit efficiency for thermoelectrics, ZT, beyond its present value for bulk materials. For reasonable parameters we estimate ZT to reach ~ 6 at room temperature.

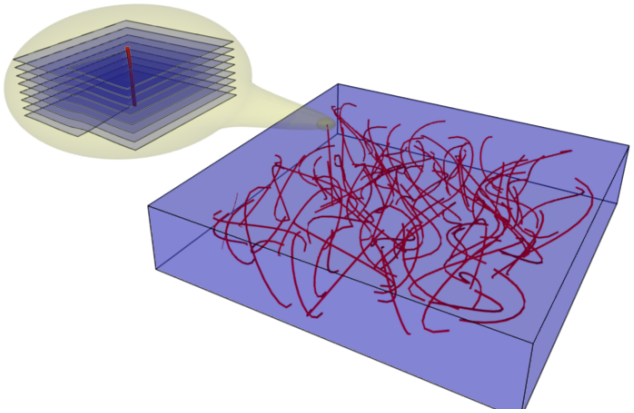

FIG. 1: (Color online) A sketch of 3D topological insulator with lattice dislocations propagating through it. These dislocations are topologically-protected 1D modes which are perfectly conducting. The inset shows the details of the screw-type dislocation considered.

Figure of merit. The performance of thermoelectric devices is determined by the dimensionless figure of merit ZT defined as

$$ZT = \frac{\sigma S^2 T}{\kappa}, \tag{1}$$

where σ, S, κ, and T are the electrical conductivity, Seebeck coefficient (or thermopower), thermal conductivity, and absolute temperature, respectively. The thermal conductivity generally has two contributions: electronic and phononic, $\kappa = \kappa_e + \kappa_{ph}$. A large effort within thermo-

electric studies is devoted to finding materials with high ZT near room temperature. The challenge is that effects that increase σ or S usually accompanies an increase on κ and vice versa. In particular, an important challenge is to reduce the phononic thermal contribution to κ which can limit severely ZT. Doing so without reducing at the same time the $\sigma S^2 T$ factor is a key challenge.

Our proposal is to exploit the 1D topological protected channels formed at the dislocations of a TI with non-zero TRIM [13] to circumvent this challenge. As more dislocations are introduced in the system the mean free path of the phonons is reduced while at the same time the conductivity contribution from the 1D channels is increased as mentioned above. By requiring that the bulk contribution is also reduced by Anderson localization of the bulk states, through the dislocations themselves or other co-doping, the ZT factor will be dominated exclusively by the 1D channels and a large ZT value can be obtained [16]. Below we present our theoretical estimate for this high ZT using reasonable estimates of the different parameters without seeking the best possible scenario but estimating instead a reasonable expectation of the proposed system.

Within linear response theory [17] the electric (j^e) and thermal (j^q) currents are given by linear combinations of the chemical potential and temperature gradients: $j^e/e = L_0\nabla\mu + L_1(\nabla T)/T$ and $j^q = -L_1\nabla\mu - L_2(\nabla T)/T$, where e is the electron charge. From these equations, using Onsager relations, one can find that the electrical conductivity $\sigma = e^2 L_0$, thermopower $S = -L_1/(eTL_0)$, and electronic thermal conductivity $\kappa_e = (L_0L_2 - L_1^2)/(TL_0)$. Then according to Eq. (1) in terms of transport coefficients L_α the figure of merit takes the form [18]:

$$ZT = \frac{(L_1^b + snL_1^{1D})^2}{(L_0^b + snL_0^{1D})(L_2^b + snL_2^{1D}) - (L_1^b + snL_1^{1D})^2 + \kappa_{ph}(L_0^b + snL_0^{1D})T}, \tag{2}$$

where n is the density of topologically-protected lattice dislocations [13], s is the cross-sectional area of the device transverse to the transport direction, and $\kappa_{ph} = \frac{c_{ph}}{3} v_{ph} l_{ph}$ is the phonon contribution to the thermal conductivity. This expression for κ_{ph} is applicable at room temperatures. In Eq. (2) it is assumed that the transport coefficients have bulk and 1D channel contributions $L_\alpha = L_\alpha^b + snL_\alpha^{1D}$, where sn gives the number of the topologically protected lattice dislocations conducting perpendicular to area s.

Next we take l_{ph} in the limit of high density of randomly located dislocations, such that for high enough dislocation density n, l_{ph} is diminished by phonon scattering from these dislocations. The phonon specific heat c_{ph} at room temperature can be estimated as $3n_i k_B$, where the number of ions per unit volume is $n_i \sim 4 \cdot 10^{29}\,\mathrm{m}^{-3}$. In $(Bi_{1-x}Sb_x)_2Te_3$ and $Bi_2(Te_{1-y}Se_y)_3$ compounds the phonon velocity $v_{ph} = 1500$ m/s and Debye temperature $\theta_D = 142$ K [19]. We also take into account in our calculations the fact that the bulk becomes an amorphous media at very high n due to disorder which leads to the saturation of κ_{ph}. Therefore, κ_{ph} ranges from $1\mathrm{Wm}^{-1}\mathrm{K}^{-1}$ for pure bulk with no dislocations [20] to $\kappa_{ph} \approx 0.01\mathrm{Wm}^{-1}\mathrm{K}^{-1}$ at average distances between dislocations $d \sim 3$ nm. It is clear from Eq. (2) that at large densities of lattice dislocations, n, the contribution to ZT mostly comes from 1D channels and in the limit equals to ZT of one perfectly conducting 1D wire:

$$\lim_{n\to\infty} ZT = \frac{(L_1^{1D})^2}{L_0^{1D}L_2^{1D} - (L_1^{1D})^2}, \tag{3}$$

To make estimates of the relative contributions of the 1D channels and bulk we model the topological Anderson insulator system as a semiconductor with one valence and one conduction band and one 1D-state corresponding to a perfectly conducting lattice dislocation (in general, one 1D-state per each dislocation), see Fig. 2 (a). We take the gap between conduction and valence bands in the bulk to be Δ ($-\Delta < E < 0$) and the transmission coefficient in the 1D channel is assumed to be unity $\mathcal{T}(E) = 1$ for simplicity. Generally $\Delta = 0.15$ eV for Bi_2Te_3 and $\Delta = 0.3$ eV for Bi_2Se_3 we use the former for our estimates. The bulk states near the edges of the band are localized with a mobility edge at E_m; this Anderson bulk localization is due to the high density of dislocations or can be induced by doping with non-magnetic impurities.

Employing the Landauer-Buttiker formalism [21, 22] we can write the expressions for the transport coefficients in the 1D channel:

$$L_\alpha^{1D} = -\frac{l}{sh}\int \mathcal{T}(E) f'(E)(E-\mu)^\alpha dE, \tag{4}$$

where l is the length of the sample in the growth direction (length of 1D channel) which has the upper limit of the inelastic coherence length ($l_{in} \sim 1\mu$m), h is a Planck constant, and $f'(E) = \partial f/\partial E$ with $f = 1/(e^{(E-\mu)/(k_BT)}+1)$ being the Fermi function. Here the integration over energies extends from $-\Delta$ to 0 while the chemical potential, which can be changed by an external gate, we restrict to be in the gap, $-\Delta < \mu < 0$, or within the conduction band, $\mu > 0$, but not much above the mobility edge. The

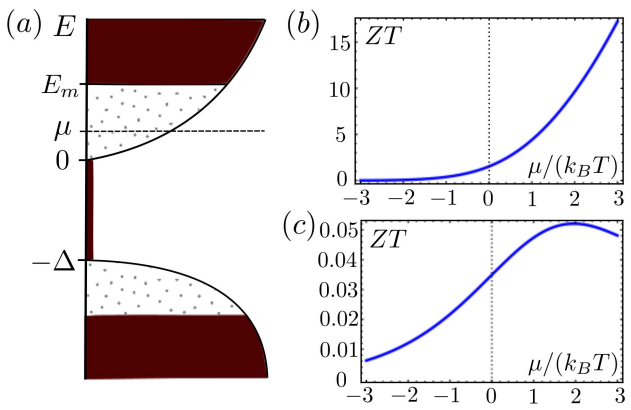

FIG. 2: (Color online) (a) Schematic band structure of the bulk and 1D states. (b) Figure of merit ZT for the contribution from topologically-protected 1D channels as a function of chemical potential μ (in units k_BT) at temperature $T = 300$ K. (c) Pure bulk contribution to ZT as a function of μ.

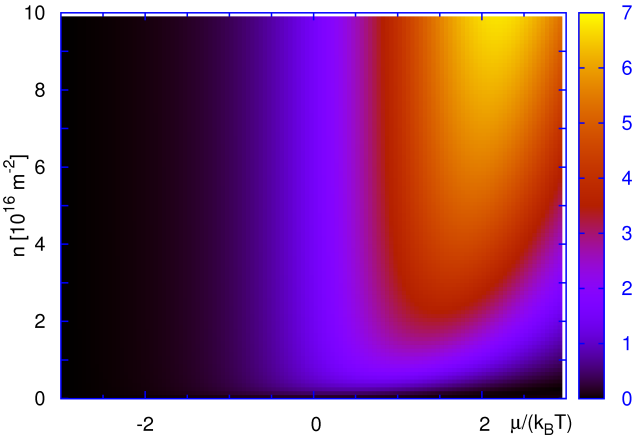

FIG. 3: (Color online) The contour plot of figure of merit ZT as a function of chemical potential μ (in units k_BT) and the density of lattice dislocations n at temperature $T = 300$ K for sample's length $l = 1\mu$m. The maximum value is higher than 6.

latter case is of the most interest, since in this case ZT is the largest, see Fig. 2 (b).

To estimate the bulk contribution to the transport coefficients L_α we assume the bands to be parabolic and use Boltzmann equation in the relaxation time approximation,

$$L^b_\alpha = -\tau \int_{E_m}^{\infty} D(E) f'(E) v^2 (E-\mu)^\alpha dE. \qquad (5)$$

Here v is electron velocity, $D(E)$ is the density of states, and we approximate relaxation time τ to be independent of energy. The extended and localized states are separated by the mobility edge E_m which is measured from the bottom of the conduction band, see Fig. 2 (a), and for further estimates we assume $E_m = 0.05$ eV. Then Eq. (5) gives

$$L^b_\alpha = \frac{2\sqrt{2m^*}}{\pi^2\hbar^3}\tau c T^{\alpha+3/2} \int_{\frac{E_m-\mu}{T}}^{\infty} dx \frac{x^\alpha (x+\mu/T)^{3/2} e^x}{(e^x+1)^2}, \qquad (6)$$

where c is the number of the carrier pockets and we take $c = 1$, $m^* = 0.02\, m_e$ is the effective mass, and temperature is measured in units of k_B. We estimate $\tau = 10^{-14}$ s. These L_α are then substituted into Eq. (2) to give ZT which is shown in Fig. 3 for a range of densities n and chemical potential μ at room temperature. The maximum, for the estimated parameters, is higher than 6, which makes these systems quite unique even if something of that order can be reached.

We note that, if the impurities are non-magnetic, the transition to a bulk Anderson insulator should not destroy the topologically protected 1D states, because the time reversal invariance is not broken. Also, note that by increasing number of dislocations or non-magnetic impurities one can come closer to the 1D wire limit for ZT and reach even greater values. These densities are however more unlikely to be achieved and can lead also to tunneling between the channels which could lead to an opening of a gap and localization of the protected states. This is the reason for our choice of an upper limit of the 1D-channel density of $n \sim 10^{17}\mathrm{m}^{-2}$ corresponding to a typical spacing of ~ 3 nm.

Summary. We have studied the thermoelectric properties of 3D topological insulators with non-zero TRIM which contain many line dislocations possessing topologically-protected perfectly conducting 1D states. We have shown that in principle this system can have very high figure of merit, $ZT \sim 10$, and predict that increasing the number of dislocations in a TI film will exhibit an increase in ZT.

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